```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

NEWS  1              Web Page URLs for STN Seminar Schedule - N. America
NEWS  2              "Ask CAS" for self-help around the clock
NEWS  3   JAN 27     Source of Registration (SR) information in REGISTRY updated
                     and searchable
NEWS  4   JAN 27     A new search aid, the Company Name Thesaurus, available in
                     CA/CAplus
NEWS  5   FEB 05     German (DE) application and patent publication number format
                     changes
NEWS  6   MAR 03     MEDLINE and LMEDLINE reloaded
NEWS  7   MAR 03     MEDLINE file segment of TOXCENTER reloaded
NEWS  8   MAR 03     FRANCEPAT now available on STN
NEWS  9   MAR 29     Pharmaceutical Substances (PS) now available on STN
NEWS 10   MAR 29     WPIFV now available on STN
NEWS 11   MAR 29     No connect hour charges in WPIFV until May 1, 2004
NEWS 12   MAR 29     New monthly current-awareness alert (SDI) frequency in RAPRA

NEWS EXPRESS  MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 13 APRIL 2004
NEWS HOURS    STN Operating Hours Plus Help Desk Availability
NEWS INTER    General Internet Information
NEWS LOGIN    Welcome Banner and News Items
NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:59:08 ON 23 APR 2004

=> file reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 09:59:15 ON 23 APR 2004
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STRUCTURE FILE UPDATES:   21 APR 2004  HIGHEST RN 676437-01-7
DICTIONARY FILE UPDATES:  21 APR 2004  HIGHEST RN 676437-01-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.
```

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> **file hcaplus**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	0.63

FILE 'HCAPLUS' ENTERED AT 09:59:19 ON 23 APR 2004
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FILE COVERS 1907 - 23 Apr 2004 VOL 140 ISS 18
FILE LAST UPDATED: 22 Apr 2004 (20040422/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> **s 126:18962/dn**
L1 1 126:18962/DN

=> **sel rn**
E1 THROUGH E22 ASSIGNED

=> **file reg**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.44	3.07

FILE 'REGISTRY' ENTERED AT 09:59:40 ON 23 APR 2004
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STRUCTURE FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7
DICTIONARY FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> s e1-e22

```
             1 14681-72-2/BI
               (14681-72-2/RN)
             1 175915-79-4/BI
               (175915-79-4/RN)
             1 184034-35-3/BI
               (184034-35-3/RN)
             1 184034-39-7/BI
               (184034-39-7/RN)
             1 184034-41-1/BI
               (184034-41-1/RN)
             1 184034-42-2/BI
               (184034-42-2/RN)
             1 184034-43-3/BI
               (184034-43-3/RN)
             1 184034-44-4/BI
               (184034-44-4/RN)
             1 184034-45-5/BI
               (184034-45-5/RN)
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             1 65490-21-3/BI
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L2          22 (14681-72-2/BI OR 175915-79-4/BI OR 184034-35-3/BI OR 184034-39-
               7/BI OR 184034-41-1/BI OR 184034-42-2/BI OR 184034-43-3/BI OR
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               7/BI OR 184034-48-8/BI OR 184034-49-9/BI OR 184034-50-2/BI OR
               184034-51-3/BI OR 184034-52-4/BI OR 184034-53-5/BI OR 184034-54-
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6/BI OR 184034-55-7/BI OR 184034-56-8/BI OR 184034-57-9/BI OR
65490-21-3/BI)

=> d can
'CAN' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats. The predefined substance formats
are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance. The substance formats
must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.

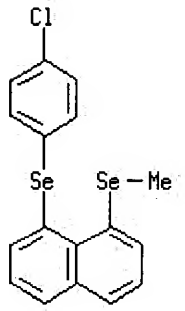
For additional information, please consult the following help
messages:

HELP DFIELDS -- To see a complete list of individual display fields.

HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):**end**

=> **d scan**

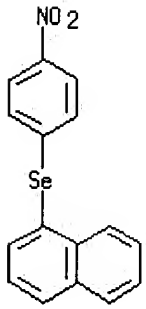
L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-[(4-chlorophenyl)seleno]-8-(methylseleno)- (9CI)
MF C17 H13 Cl Se2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

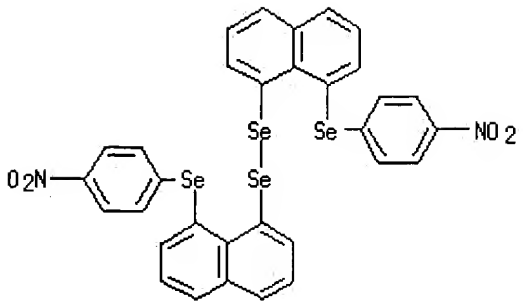
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1)**22**

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-[(4-nitrophenyl)seleno]- (9CI)
MF C16 H11 N O2 Se



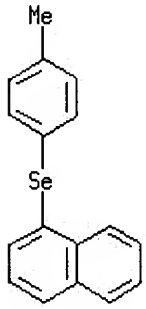
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Diselenide, bis[8-[(4-nitrophenyl)seleno]-1-naphthalenyl] (9CI)
MF C32 H20 N2 O4 Se4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

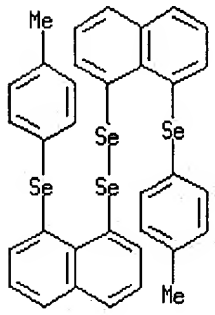
L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-[(4-methylphenyl)seleno]- (9CI)
MF C17 H14 Se



102 (b)

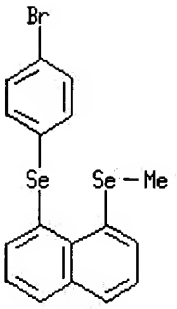
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Diselenide, bis[8-[(4-methylphenyl)seleno]-1-naphthalenyl] (9CI)
MF C34 H26 Se4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-[(4-bromophenyl)seleno]-8-(methylseleno)- (9CI)
MF C17 H13 Br Se2

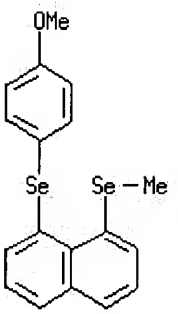


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Selenium, isotope of mass 77 (8CI, 9CI)
MF Se

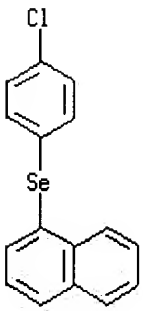
^{77}Se

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-[(4-methoxyphenyl)seleno]-8-(methylseleno)- (9CI)
MF C18 H16 O Se2



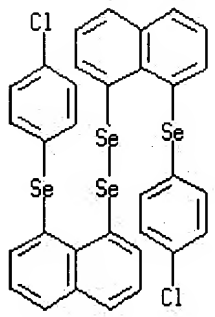
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-[(4-chlorophenyl)seleno]- (9CI)
MF C16 H11 Cl Se



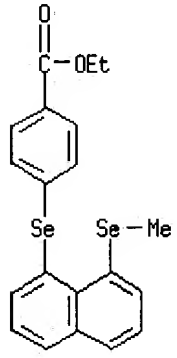
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Diselenide, bis[8-[(4-chlorophenyl)seleno]-1-naphthalenyl] (9CI)
MF C32 H20 Cl2 Se4



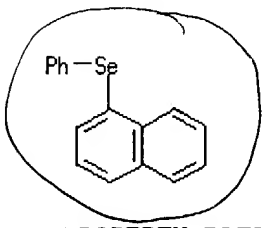
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzoic acid, 4-[[8-(methylseleno)-1-naphthalenyl]seleno]-, ethyl ester (9CI)
MF C20 H18 O2 Se2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

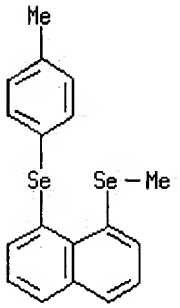
L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-(phenylseleno)- (9CI)
MF C16 H12 Se



103(a) bioisostere H is isostere of R_1 = methyl

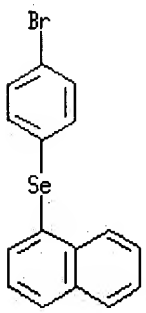
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-[(4-methylphenyl)seleno]-8-(methylseleno)- (9CI)
MF C18 H16 Se2



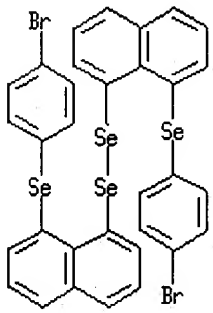
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-[(4-bromophenyl)seleno]- (9CI)
MF C16 H11 Br Se



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

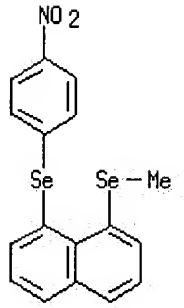
L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Diselenide, bis[8-[(4-bromophenyl)seleno]-1-naphthalenyl] (9CI)
MF C32 H20 Br2 Se4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

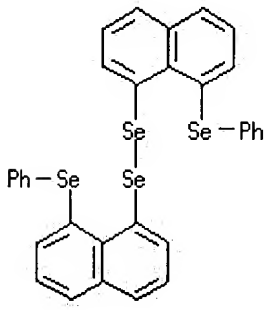
L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-(methylseleno)-8-[(4-nitrophenyl)seleno]- (9CI)

MF C17 H13 N O2 Se2



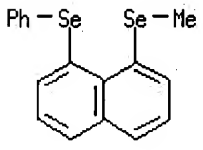
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Diselenide, bis[8-(phenylseleno)-1-naphthalenyl] (9CI)
MF C32 H22 Se4



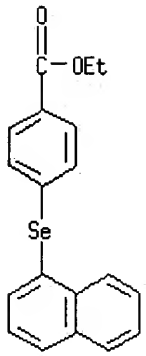
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-(methylseleno)-8-(phenylseleno)- (9CI)
MF C17 H14 Se2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

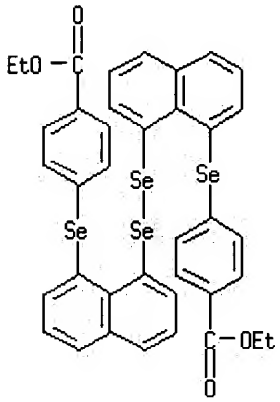
L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzoic acid, 4-(1-naphthalenylseleno)-, ethyl ester (9CI)
MF C19 H16 O2 Se



103(a) Esters obvious on Carboxylic Acids
Prior

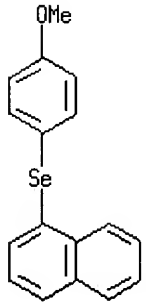
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzoic acid, 4,4'-[diselenobis(8,1-naphthalenediylseleno)]bis-, diethyl ester (9CI)
MF C38 H30 O4 Se4



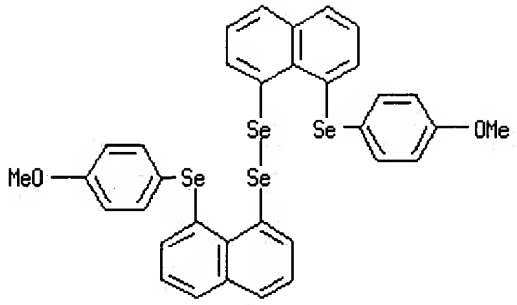
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Naphthalene, 1-[(4-methoxyphenyl)seleno]- (9CI)
MF C17 H14 O Se



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 22 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Diselenide, bis[8-[(4-methoxyphenyl)seleno]-1-naphthalenyl] (9CI)
MF C34 H26 O2 Se4

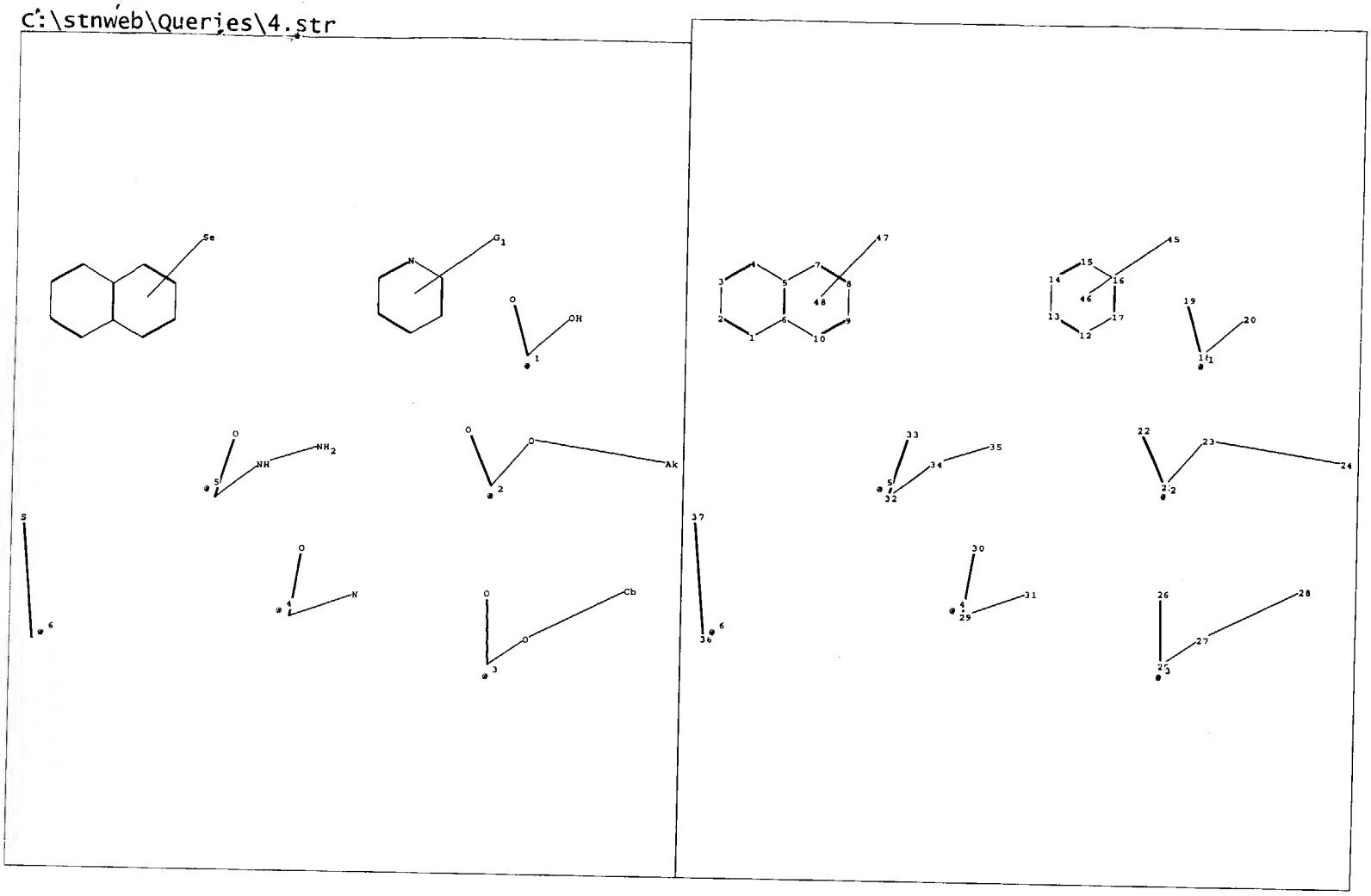


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>

C:\stnweb\Queries\4.str

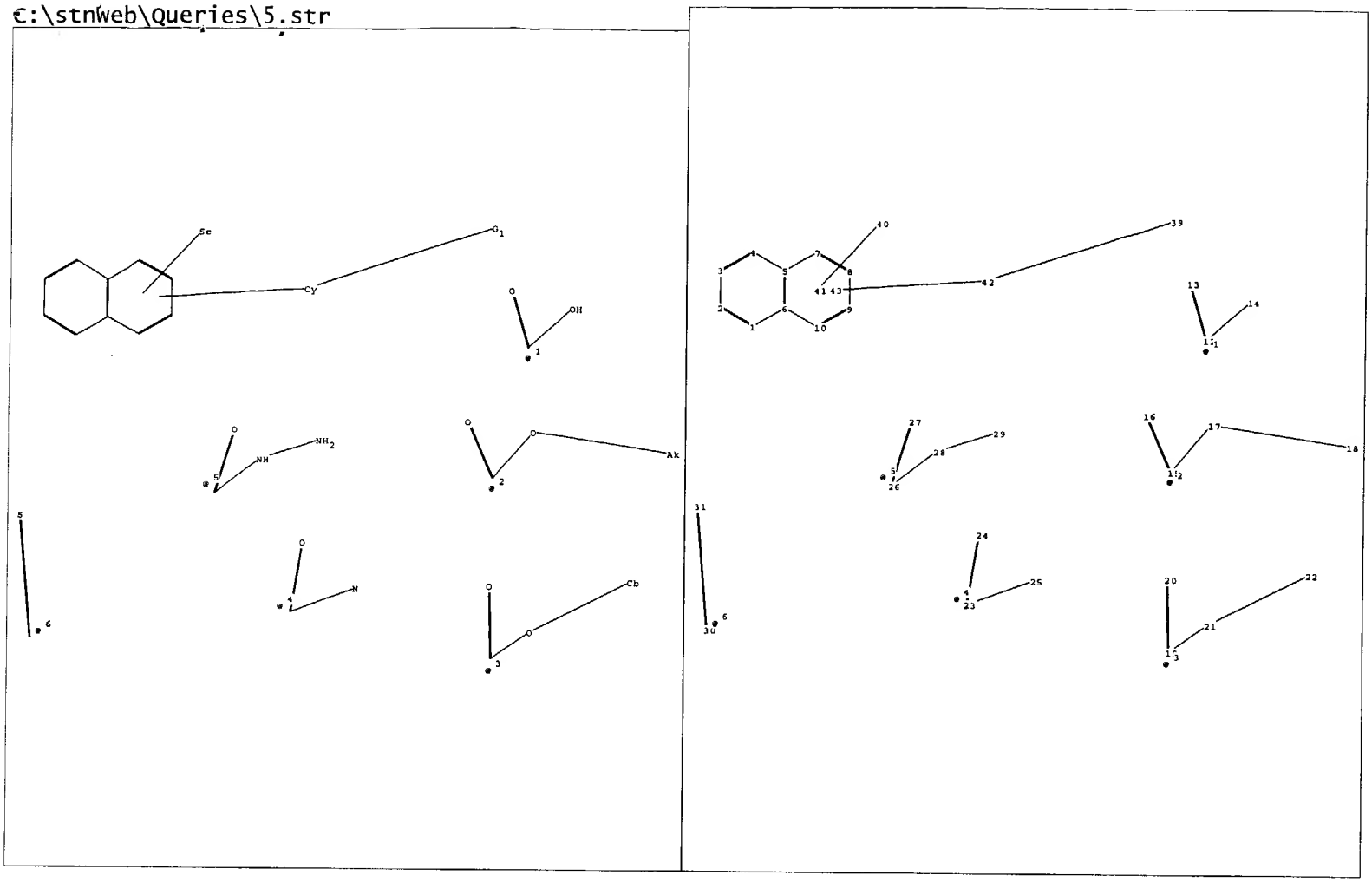


chain nodes :
18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 45 47
ring nodes :
1 2 3 4 5 6 7 8 9 10 12 13 14 15 16 17
chain bonds :
18-19 18-20 21-22 21-23 23-24 25-26 25-27 27-28 29-30 29-31 32-33 32-34 34-35
36-37
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-17 13-14 14-15 15-16
16-17
exact/norm bonds :
21-22 21-23 23-24 25-26 25-27 29-30 29-31 32-33 32-34 36-37
exact bonds :
27-28 34-35
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-17 13-14 14-15 15-16
16-17 18-19 18-20
isolated ring systems :
containing 1 : 12 :

G1:[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:Atom 29:CLASS 30:CLASS
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 45:CLASS 46:CLASS
47:CLASS 48:CLASS

C:\stnweb\Queries\5.str

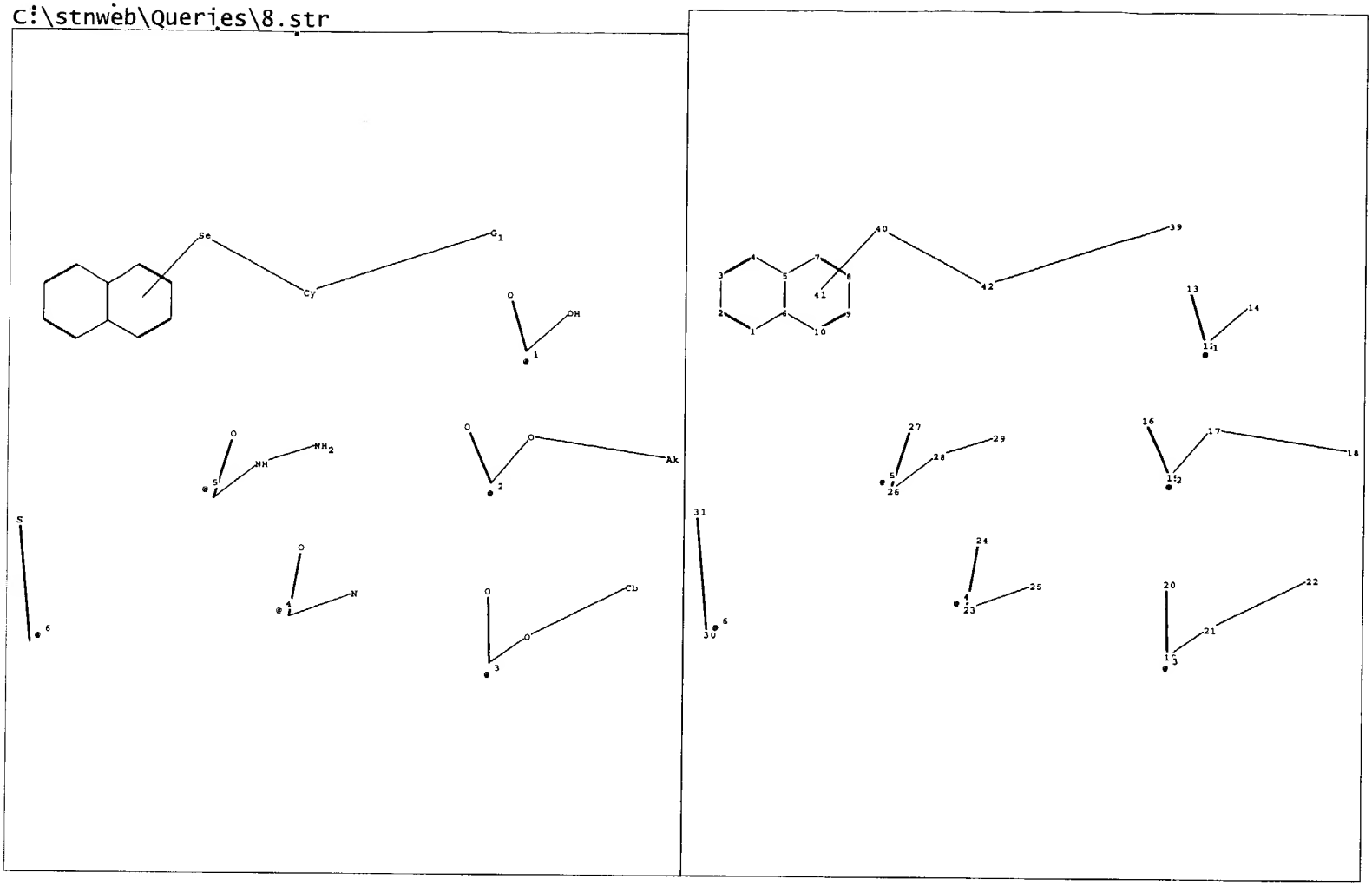


chain nodes :
12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 39 40 42
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
12-13 12-14 15-16 15-17 17-18 19-20 19-21 21-22 23-24 23-25 26-27 26-28 28-29
30-31 39-42
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
15-16 15-17 17-18 19-20 19-21 23-24 23-25 26-27 26-28 30-31 39-42
exact bonds :
21-22 28-29
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-14
isolated ring systems :
containing 1 :

G1:[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:CLASS

C:\stnweb\Queries\8.str

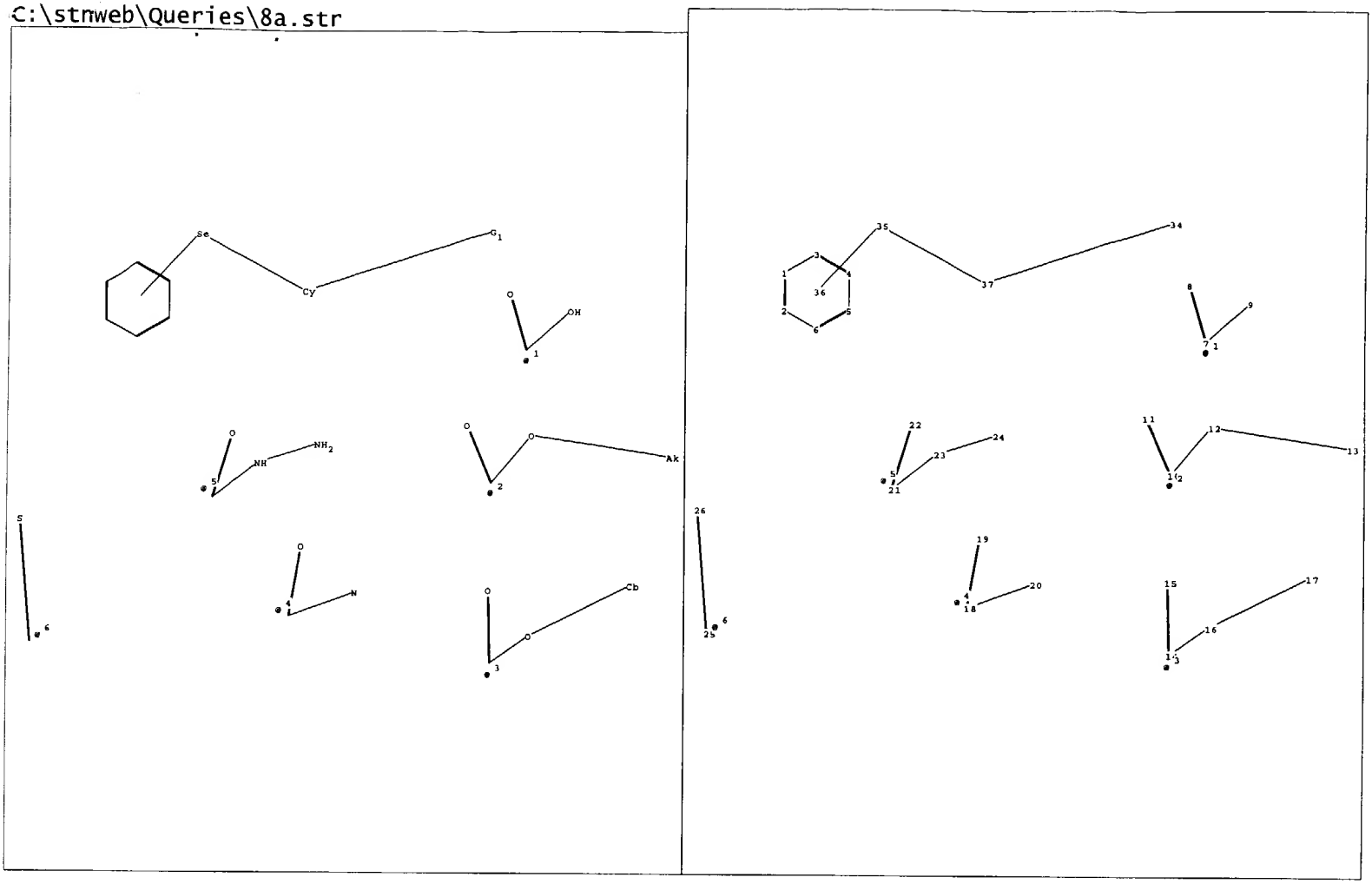


chain nodes :
12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 39 40 42
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
12-13 12-14 15-16 15-17 17-18 19-20 19-21 21-22 23-24 23-25 26-27 26-28 28-29
30-31 39-42 40-42
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
15-16 15-17 17-18 19-20 19-21 23-24 23-25 26-27 26-28 30-31 39-42 40-42
exact bonds :
21-22 28-29
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-14
isolated ring systems :
containing 1 :

G1:[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom

C:\stnweb\Queries\8a.str

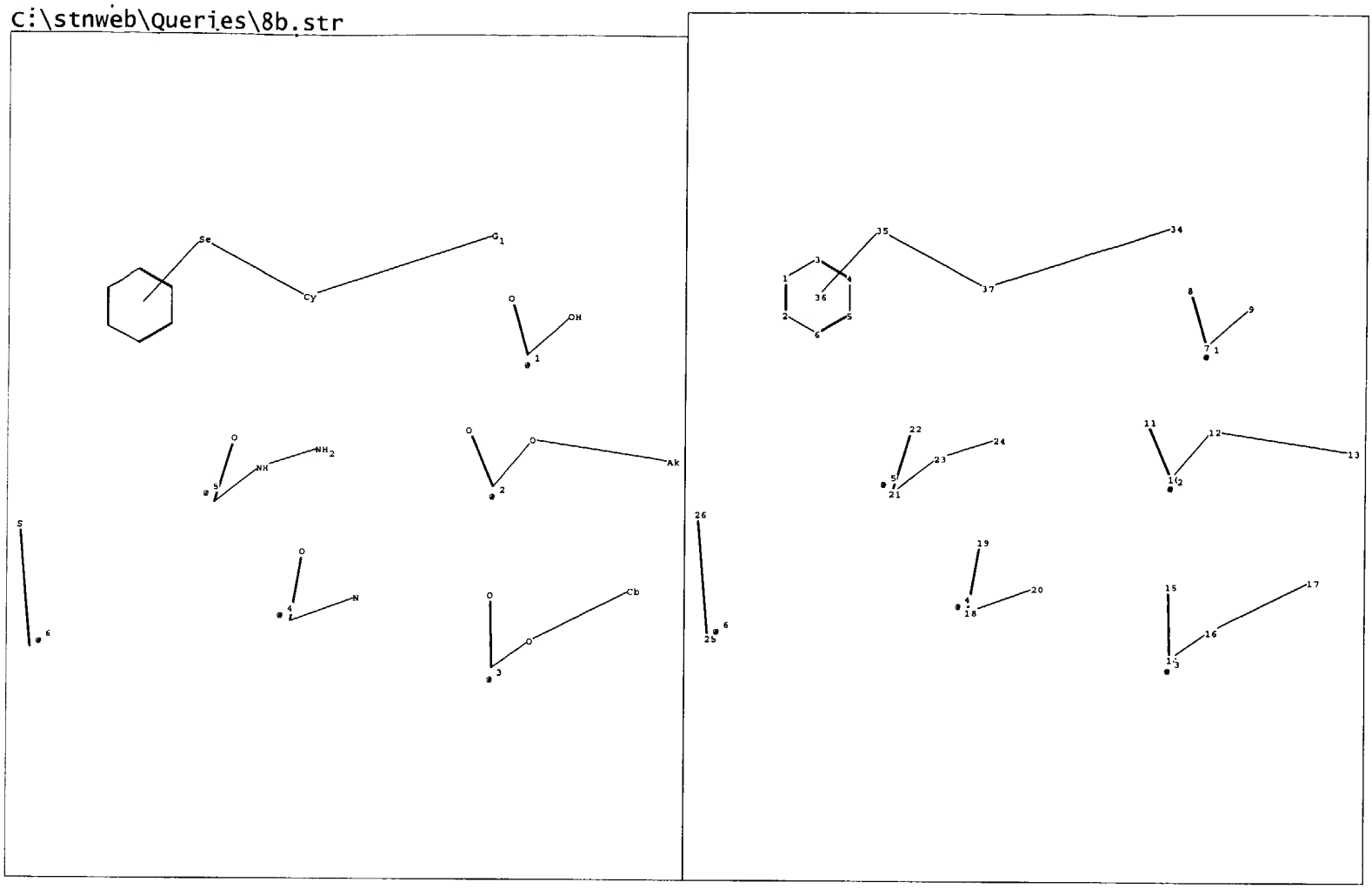


chain nodes :
7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 34 35 37
ring nodes :
1 2 3 4 5 6
chain bonds :
7-8 7-9 10-11 10-12 12-13 14-15 14-16 16-17 18-19 18-20 21-22 21-23 23-24
25-26 34-37 35-37
ring bonds :
1-3 1-2 2-6 3-4 4-5 5-6
exact/norm bonds :
10-11 10-12 12-13 14-15 14-16 18-19 18-20 21-22 21-23 25-26 34-37 35-37
exact bonds :
16-17 23-24
normalized bonds :
1-3 1-2 2-6 3-4 4-5 5-6 7-8 7-9

G1:[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 34:CLASS 35:CLASS
36:CLASS 37:Atom

C:\stnweb\Queries\8b.str



chain nodes :
7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 34 35 37
ring nodes :
1 2 3 4 5 6
chain bonds :
7-8 7-9 10-11 10-12 12-13 14-15 14-16 16-17 18-19 18-20 21-22 21-23 23-24
25-26 34-37 35-37
ring bonds :
1-3 1-2 2-6 3-4 4-5 5-6
exact/norm bonds :
10-11 10-12 12-13 14-15 14-16 18-19 18-20 21-22 21-23 25-26 34-37 35-37
exact bonds :
16-17 23-24
normalized bonds :
1-3 1-2 2-6 3-4 4-5 5-6 7-8 7-9
isolated ring systems :
containing 1 :

G1:[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 34:CLASS 35:CLASS
36:CLASS 37:Atom

```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

NEWS  1              Web Page URLs for STN Seminar Schedule - N. America
NEWS  2              "Ask CAS" for self-help around the clock
NEWS  3   JAN 27     Source of Registration (SR) information in REGISTRY updated
                     and searchable
NEWS  4   JAN 27     A new search aid, the Company Name Thesaurus, available in
                     CA/CAplus
NEWS  5   FEB 05     German (DE) application and patent publication number format
                     changes
NEWS  6   MAR 03     MEDLINE and LMEDLINE reloaded
NEWS  7   MAR 03     MEDLINE file segment of TOXCENTER reloaded
NEWS  8   MAR 03     FRANCEPAT now available on STN
NEWS  9   MAR 29     Pharmaceutical Substances (PS) now available on STN
NEWS 10   MAR 29     WPIFV now available on STN
NEWS 11   MAR 29     No connect hour charges in WPIFV until May 1, 2004
NEWS 12   MAR 29     New monthly current-awareness alert (SDI) frequency in RAPRA

NEWS EXPRESS  MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 13 APRIL 2004
NEWS HOURS    STN Operating Hours Plus Help Desk Availability
NEWS INTER    General Internet Information
NEWS LOGIN    Welcome Banner and News Items
NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:28:14 ON 23 APR 2004

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     1.47       1.47

FILE 'REGISTRY' ENTERED AT 09:32:24 ON 23 APR 2004
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STRUCTURE FILE UPDATES:   21 APR 2004  HIGHEST RN 676437-01-7
DICTIONARY FILE UPDATES:  21 APR 2004  HIGHEST RN 676437-01-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.
```

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

=> s l1
SAMPLE SEARCH INITIATED 09:42:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 6 TO 266
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:42:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 83 TO ITERATE

100.0% PROCESSED 83 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> file beilstein
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 162.56 164.03

FILE 'BEILSTEIN' ENTERED AT 09:42:55 ON 23 APR 2004
COPYRIGHT (c) 2004 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON MARCH 30,2004

FILE COVERS 1771 TO 2003.
FILE CONTAINS 8,932,479 SUBSTANCES

>>> PLEASE NOTE: Reaction data and substance data are stored in separate documents and can not be searched together in one query.
Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA

(reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

```
**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE   *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE          *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                        *
* FOR PRICE INFORMATION SEE HELP COST                                *
**********************************************************************
```

=> **d his**

(FILE 'HOME' ENTERED AT 09:28:14 ON 23 APR 2004)

FILE 'REGISTRY' ENTERED AT 09:32:24 ON 23 APR 2004

```
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FULL
```

FILE 'BEILSTEIN' ENTERED AT 09:42:55 ON 23 APR 2004

=> **s l1**

```
SAMPLE SEARCH INITIATED 09:43:02 FILE 'BEILSTEIN'
SAMPLE SCREEN SEARCH COMPLETED -      0 TO ITERATE

100.0% PROCESSED       0 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            0 TO        0
PROJECTED ANSWERS:               0 TO        0

L4           0 SEA SSS SAM L1
```

=> **file reg**

```
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.06     164.09

FILE 'REGISTRY' ENTERED AT 09:43:07 ON 23 APR 2004
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provided by InfoChem.

STRUCTURE FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7
DICTIONARY FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L5 STRUCTURE UPLOADED

=> **d l5**
L5 HAS NO ANSWERS
L5 STR

=> **s l5**
SAMPLE SEARCH INITIATED 09:44:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED 29 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 257 TO 903
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> **s l5 full**
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:44:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 570 TO ITERATE

100.0% PROCESSED 570 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L7 0 SEA SSS FUL L5

=>
L8 STRUCTURE UPLOADED

=> l8
L8 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> **d l8**
L8 HAS NO ANSWERS

```
L8              STR

=> s l8
SAMPLE SEARCH INITIATED 09:45:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     29 TO ITERATE

100.0% PROCESSED      29 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          257 TO      903
PROJECTED ANSWERS:               0 TO        0

L9            0 SEA SSS SAM L8

=> s l8 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:45:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     570 TO ITERATE

100.0% PROCESSED     570 ITERATIONS                                 10 ANSWERS
SEARCH TIME: 00.00.01

L10           10 SEA SSS FUL L8

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   312.10     476.19

FILE 'HCAPLUS' ENTERED AT 09:45:49 ON 23 APR 2004
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FILE COVERS 1907 - 23 Apr 2004  VOL 140 ISS 18
FILE LAST UPDATED: 22 Apr 2004  (20040422/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l10
L11           7 L10

=> s l11 and bernardon, J?/au
            68 BERNARDON, J?/AU
```

```
L12             0 L11 AND BERNARDON, J?/AU

=> s l11 and diaz, p?/au
            602 DIAZ, P?/AU
L13             0 L11 AND DIAZ, P?/AU

=> d l11, ibib abs fhitstr, 1-7

L11  ANSWER 1 OF 7  HCAPLUS  COPYRIGHT 2004 ACS on STN
```

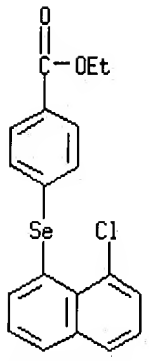
Full Text | Citing References

ACCESSION NUMBER: 2001:899884 HCAPLUS
DOCUMENT NUMBER: 136:183576
TITLE: Structure of 1-(Arylselenyl)naphthalenes. 2. G Dependence in 8-G-1-(p-YC6H4Se)C10H6
AUTHOR(S): Nakanishi, Waro; Hayashi, Satoko
CORPORATE SOURCE: Department of Chemistry and Materials Science Faculty of Systems Engineering, Wakayama University, Sakaedani Wakayama, 640-8510, Japan
SOURCE: Journal of Organic Chemistry (2002), 67(1), 38-48
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:183576

AB The structures of 8-G-1-(p-YC6H4Se)C10H6 (1 (G = Cl) and 2 (G = Br): Y = H (a), OMe (b), Me (c), Cl (d), Br (e), COOEt (f), and NO2 (g)) were investigated by x-ray crystallog. anal., NMR spectroscopy, and ab initio MO calcns. The structures of all members in 1 and 2 are concluded to be type B, which is in striking contrast to the type A structure for 4d-g (4 (g(n)), where G = H). The Se-Ci bond of the p-YC6H4Se group in 8-G-1-(p-YC6H4Se)C10H6 is almost perpendicular to the naphthyl plane in type A, and it is located on the plane in type B. The chlorine and bromine substitution at the 8-position in 1 and 2 dramatically changes the type A structure of 4 (g(n)) to type B. The nonbonded G- - -Se-C 3c-4e type interaction must contribute to stabilize the type B structure. The type B structure in 1 and 2 should also be more stabilized than the same structure in 4 by the 3c-4e type interaction: The structure of 4b is type B in the crystals and type B would be more stable for 4c and might be for 4a in solns. Ab initio MO calcns. are performed on 8-G-1-(p-YC6H4Se)C10H6, 8-G-C10H6SeH-1, and models HG- - -SeH2, where G = Cl, Br, and F, to clarify the reason for the dramatic change in the structures. The type B structure is optimized to be more stable than the type A for all species examd., which supports the observations. The energy differences between type B and type A are larger for the models than for the naphthalenes. While the superiority of the type B for the former is Br > Cl » F, that of the latter is Br ≈ Cl ≥ F.
These results show that the main factor of the structural change from type A to type B is the nonbonded G- - -Se-C 3c-4e interaction. The electronic effect of halogens through the naphthalene π-framework would also contribute to some extent, although the direct comparison of the evaluated values between the naphthalene systems and the models is not so easy. Factors to stabilize the two structures of 1, 2, 4, and 8-(MeSe)-1-(p-YC6H4Se)C10H6 are reexamd. from a viewpoint of the nonbonded G- - -Se-C 3c-4e interaction (G dependence), together with the electronic effect of Y (Y dependence).

IT **399509-44-5P**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(prepn. and ab initio MO calcn. of)
RN 399509-44-5 HCAPLUS
CN Benzoic acid, 4-[(8-chloro-1-naphthalenyl)seleno]-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:790438 HCAPLUS
DOCUMENT NUMBER: 136:199813
TITLE: Structure of 1-(arylselanyl)naphthalenes - Y dependence in 1-(p-YC6H4Se)C10H7
AUTHOR(S): Nakanishi, Waro; Hayashi, Satoko; Uehara, Tetsutaro
CORPORATE SOURCE: Department of Material Science and Chemistry, Faculty of Systems Engineering, Wakayama University, Wakayama, 640-8510, Japan
SOURCE: European Journal of Organic Chemistry (2001), (20), 3933-3943
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

= Examine for operability

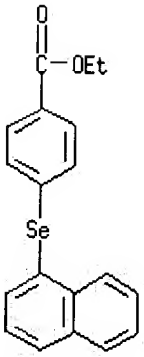
AB The structures of 1-(arylselanyl)naphthalenes, 1-(p-YC6H4Se)C10H7 [I, Y = H, OMe, Me, Cl, Br, CO2Et, NO2] were detd. The structures of I were well classified using types A, B, and C, where the Se-CAr bond is placed almost perpendicular to the naphthyl plane in type A and is located on the plane in type B. The type C structure is intermediate between type A and type B. The structures of I [Y = Cl, Br, CO2Et] are demonstrated to be type A whereas that of I [Y = OMe] is type B by X-ray crystallog. anal. The type B conformer is suggested to be favorable in solns. for I [Y = H, Me] based on the NMR-spectroscopic data. The structure of I [Y = NO2] is assumed to be type A. These results show that the stable structure of I must be type A or type B, contrary to early observations of type C for 1,8-bis(alkyl- or arylchalcogeno)naphthalenes. Consequently, the solid state structure of I changes dramatically depending on Y. It is proposed that these structures can be explained by the electron affinities, together with the energies of LUMO and LUMO+1 of benzene, substituted benzene, and naphthalene, which are the components of I. In order to clarify the reason for the dramatic change in the structure of I with change in Y, ab initio MO calcns. were performed on I and related compds. The type A and type B conformations were optimized as stable mols. Although I [Y = H] (type A) is predicted to be more stable than I [Y = H] (type B) by 1.3 kJ mol-1, the latter becomes more stable than the former by 8.4 kJ mol-1 if the solvent effects of chloroform are taken into account in the calcns.,

which was done by applying the IPCM method. The transition state between type A and type B in I [Y = H] is similar to type C, which must prevent the monotonic change in the structure of I. I would be in equil. between type A and type B in solns. The results of the MO calcns. on I suggest that type A is exclusive for I [Y = NO2], and probably exclusive for I [Y = CO2Et], and predominant for I [Y = Cl, Br], while type B is predominant for I [Y = OMe]. Type A and type B would be comparable for I [Y = H, Me].

IT **184034-56-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and substituent effect on the structure of 1-(arylselanyl)naphthalenes)

RN 184034-56-8 HCAPLUS

CN Benzoic acid, 4-(1-naphthalenylseleno)-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:505214 HCAPLUS
DOCUMENT NUMBER: 131:271940
TITLE: Novel Substituent Effect on 77Se NMR Chemical Shifts Caused by 4c-6e versus 2c-4e and 3c-4e in Naphthalene Peri Positions: Spectroscopic and Theoretical Study
AUTHOR(S): Hayashi, Satoko; Nakanishi, Waro
CORPORATE SOURCE: Department of Material Science and Chemistry Faculty of Systems Engineering, Wakayama University, Wakayama, 640-8510, Japan
SOURCE: Journal of Organic Chemistry (1999), 64(18), 6688-6696
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB δ(8Se) values for 1-[8-(p-YC6H4Se)C10H6]SeSe[C10H6(SeC6H4Y-p)-8']-1' (1: Y = H, OMe, Me, Cl, Br, COOEt, and NO2) showed a good correlation with those of 1-(MeSe)-8-(p-YC6H4Se)C10H6 (2). While the δ(1Se) values correlated well with δ(8Se) in 2 with a pos. proportionality const. of 0.252 (regular correlation), a similar correlation for 1 gave a neg. proportionality const. of -0.282 (inverse correlation). To clarify the mechanism assocd. with the inverse correlation in 1, together with the regular correlation in 2, ab initio MO calcns., contg. the GIAO magnetic shielding tensor for the Se nucleus (σ(Se)), were performed on p-YC6H4ASeH- - -BSeH-BSeH- - -HASeC6H4Y-p (3: model of Se4 4c-6e for 1) and on p-YC6H4ASeH- - -BSeH2 (4 and 5: models of Se2 π type 2c-4e and

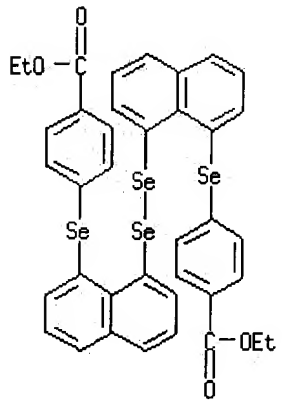
ASe- - -BSe-H 3c-4e for 2, resp.) with the 6-311+G(2d,p) basis sets at B3LYP and/or HF levels. The characteristic nature of the substituent effects on at. charges and δ(Se) values in 3 is demonstrated to be Yδ-←C6H4-Seδ+- - -Seδ+-Seδ+- - -Seδ+-C6H4→Yδ- and Yδ-←C6H4-Sedown- - -Seup-Seup- - -Sedown-C6H4→Yδ-, resp., (Y = electron-withdrawing) and in 5 is Yδ-←C6H4-Seδ+- - -Seδ--Hδ+ and Yδ-←C6H4-Sedown- - -Sedown-Hdown, resp. In the case of 4, a substantial contribution through the naphthylidene group is suggested. These results indicate that the nature of the interaction between the linear four Se atoms in 1 is of the 4c-6e type and that between the two Se atoms in 2 is π type 2c-4e and/or 3c-4e according to the conformations around the Se atoms. The obsd. NMR parameters are well explained by model calcns. on 3-5. Plots of 4J(1Se,8Se) vs. δ(8Se) of 1 and 2 gave good correlations with neg. proportionality consts., which indicates that the J values become larger as the electron d. on the 8Se atoms increases.

IT **184034-43-3P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(spectroscopic and theor. study of novel substituent effect on selenium NMR chem. shifts caused by 4center-6electron vs. 2center-4electron and 3center-4electron in naphthalene peri positions)

RN 184034-43-3 HCAPLUS

CN Benzoic acid, 4,4'-[diselenobis(8,1-naphthalenediylseleno)]bis-, diethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

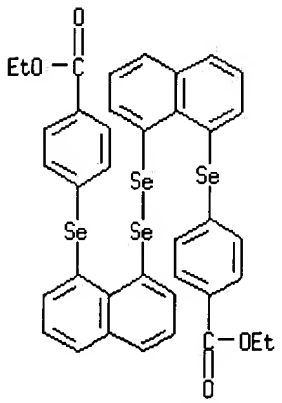
ACCESSION NUMBER: 1999:439061 HCAPLUS
DOCUMENT NUMBER: 131:228777
TITLE: Structural Study of Aryl Selenides in Solution Based on 77Se NMR Chemical Shifts: Application of the GIAO Magnetic Shielding Tensor of the 77Se Nucleus
AUTHOR(S): Nakanishi, Waro; Hayashi, Satoko
CORPORATE SOURCE: Department of Material Science and Chemistry Faculty of Systems Engineering, Wakayama University, Sakaedani Wakayama, 640-8510, Japan
SOURCE: Journal of Physical Chemistry A (1999), 103(31), 6074-6081

CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The 77Se NMR chem. shifts (δobsd(Se)) of p-YC6H4SeMe (1: Y = H (a), OMe (b), Me (c), Cl (d), Br (e), COOR (f), and NO2 (g)) and p-YC6H4SePh (2) were detd. or redetd. in chloroform-d. The δobsd(Se) values of 2, p-YC6H4SeR [R = CN (3), Bz (4), H (5), Br (6), Et (7), C6H4Y-p (8), CH:CH2 (9), CH:CHCl-t (10), and CHCH2CCl2-cyclo (11)], 1,1'-[8-(p-YC6H4Se)C10H6Se]2 (12), and 1-(MeSe)-8-(p-YC6H4Se)C10H6 (13) were plotted against those of 1. The plots were analyzed as two correlations. For example, the points corresponding to a-c make a group (g(m)), and those of d-g belong to another one (g(n)). This must be a reflection of the differences in the dihedral angles between the aryl rings and the Se-R bonds, which should result in the different contributions of the inductive and mesomeric effects of the substituents Y on the δobsd(Se) values. After reexamn. of the applicability of the GIAO magnetic shielding tensor for the Se nucleus (σ(Se)) in Se compds. of various structures, σ(Se) was calcd. for the model compds., 5, with the B3LYP/6-311+G(d,p) method, to explain the δobsd(Se) values of 1-13 uniformly: δcalcd(Se) was defined as -(σ(Se) - σ(Se)MeSeMe). Each selenol was optimized to be the planar structure (14) or the perpendicular one (15). New parameters were devised such as δcalcd(Se:θB) = (1 - sin θB)δcalcd(Se)14 + sin (θB)δcalcd(Se)15. The δobsd(Se) values of 1-13 correlated well with the new parameters, δcalcd(Se:θB), which gave the best-fitted θB values. The structures of 1-13 in solns. were explained uniformly by the evaluated θB values. The obsd. ratios of the slopes for g(m) vs. those of g(n) were also correlated with the θB values.

IT **184034-43-3**
RL: PRP (Properties)
(structural study of aryl selenides in soln. based on Se NMR chem. shifts and application of the GIAO magnetic shielding tensor of the 77Se nucleus)

RN 184034-43-3 HCAPLUS
CN Benzoic acid, 4,4'-[diselenobis(8,1-naphthalenediylseleno)]bis-, diethyl ester (9CI) (CA INDEX NAME)

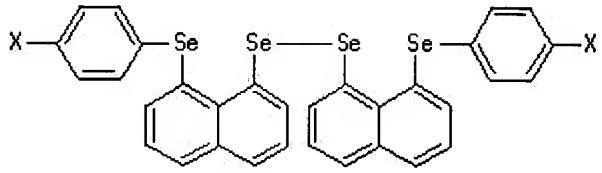


REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1996:680465 HCAPLUS
DOCUMENT NUMBER: 126:18962
TITLE: Inverse substituent effect on 77Se NMR chemical shifts in naphthalene systems with linear 4c-6e Se4 bond: 1-[8-(p-YC6H4Se)C10H6]SeSe[C10H6(SeC6H4Y-p)-8']-1' vs. 1-(MeSe)-8-(p-YC6H4Se)C10H6
AUTHOR(S): Nakanishi, Waro; Hayashi, Satoko; Yamaguchi, Hitomi
CORPORATE SOURCE: Dep. Chem., Wakayama Univ., Wakayama, 640, Japan
SOURCE: Chemistry Letters (1996), (11), 947-948
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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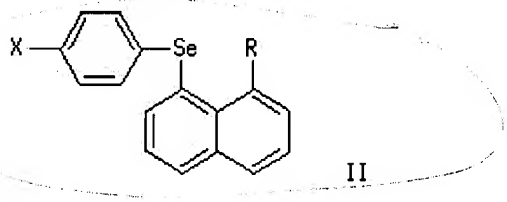


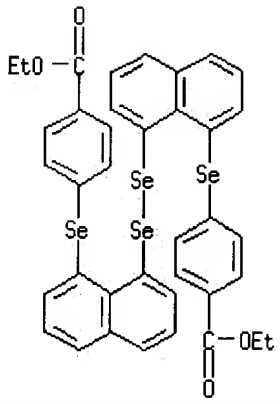
II

103(a)

AB The substituent effect on δ(1Se) vs. δ(8Se) in bis[8-(arylselanyl)naphthyl] diselenides (I, X = OMe, Me, H, Cl, Br, CO2Et, NO2) was opposite to that for 1-(methylselenyl)-8-(phenylselenyl)naphthalene II (R = SeMe, H) and its p-substituted derivs. The observation must be the reflection of the 4c-6e interaction between the p-orbitals of the four Se atoms in I.

IT **184034-43-3**
RL: PRP (Properties)
(selenium-77 NMR chem. shifts and an inverse substituent effect)
RN 184034-43-3 HCAPLUS
CN Benzoic acid, 4,4'-[diselenobis(8,1-naphthalenediylseleno)]bis-, diethyl ester (9CI) (CA INDEX NAME)

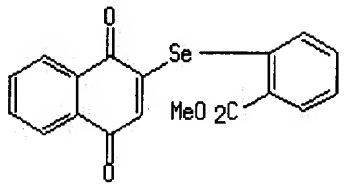
Protected Group = 103(a)
also 103(a) for Genus



L11 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1992:571583 HCAPLUS
DOCUMENT NUMBER: 117:171583
TITLE: Efficient selenation of quinones: synthesis of novel benzo[b]naphtho[2,3-e]selenintrione and dibenzo[b,e]seleninone
AUTHOR(S): Sakakibara, Makoto; Toru, Takeshi; Imai, Takahiro; Watanabe, Yoshihiko; Ueno, Yoshio
CORPORATE SOURCE: Dep. Appl. Chem., Nagoya Inst. Technol., Nagoya, 466, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1992), 65(5), 1291-4
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:171583
GI



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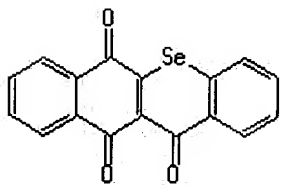
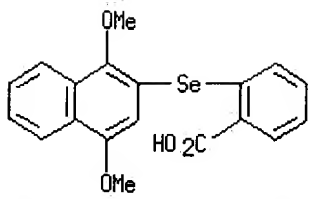


II

AB Selenation of 2-bromonaphthoquinone with an areneselenolate ion generated from (2-MeO2CC6H4)2Se2, Ph2PCl, and LiOH afforded 2-[[2-(methoxycarbonyl)phenyl]seleno]-1,4-naphthoquinone (I), from which 12H-benzo[b]naphtho[2,3-e]selenin-6,11,12-trione (II) was synthesized in 5 steps. 1,4-Dimethoxy-2,3-dimethyl-10H-dibenzo[b,e]selenin-10-one was prepd. starting from 6-bromo-2,3-dimethylbenzoquinone through the selenation and cyclization steps.

IT **143716-11-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of)

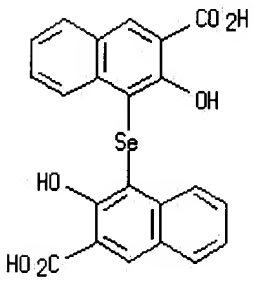
RN 143716-11-4 HCAPLUS
CN Benzoic acid, 2-[(1,4-dimethoxy-2-naphthalenyl)seleno]- (9CI) (CA INDEX NAME)



L11 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1957:22650 HCAPLUS
DOCUMENT NUMBER: 51:22650
ORIGINAL REFERENCE NO.: 51:4559e-h
TITLE: Anti-tumor substances. I. Effect of some organic selenium compounds on the Ehrlich ascites carcinoma
AUTHOR(S): Takeda, Kenichi; Nishimura, Haruo; Shimaoka, Noboru; Noguchi, Ranko; Nakajima, Kiyoshi
CORPORATE SOURCE: Shionogi Research Lab., Amagasaki, Hyogo
SOURCE: Ann. Rept. Shionogi Research Lab. (1955), 5, 1-16
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Ten kinds of org. Se compds. were synthesized and their actions on the intraperitoneal Ehrlich ascitic form of tumors were tested. Of these compds. the following were active: 5,6-dihydro-5,5-dimethyl-4H-2,1,3-benzoxaselenazol-7(7aH)-one oxime, benzoselenazole-1/2H2SO4, I and II. II is most active, superior even to nitrogen-mustard N-oxide. The effect of compds. on the intraperitoneal Ehrlich ascitic form is a particularly satisfactory way to obtain the S.D.50 in screening tests.
IT **119248-56-5**, 2-Naphthoic acid, 4,4'-selenobis[3-hydroxy-
(effect on carcinoma)
RN 119248-56-5 HCAPLUS
CN 2-Naphthoic acid, 4,4'-selenobis[3-hydroxy- (6CI) (CA INDEX NAME)



=> **file caold**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	35.66	511.85
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.85	-4.85

FILE 'CAOLD' ENTERED AT 09:46:38 ON 23 APR 2004
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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=> d his

     (FILE 'HOME' ENTERED AT 09:28:14 ON 23 APR 2004)

     FILE 'REGISTRY' ENTERED AT 09:32:24 ON 23 APR 2004
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FULL

     FILE 'BEILSTEIN' ENTERED AT 09:42:55 ON 23 APR 2004
L4           0 S L1

     FILE 'REGISTRY' ENTERED AT 09:43:07 ON 23 APR 2004
L5             STRUCTURE UPLOADED
L6           0 S L5
L7           0 S L5 FULL
L8             STRUCTURE UPLOADED
L9           0 S L8
L10         10 S L8 FULL

     FILE 'HCAPLUS' ENTERED AT 09:45:49 ON 23 APR 2004
L11          7 S L10
L12          0 S L11 AND BERNARDON, J?/AU
L13          0 S L11 AND DIAZ, P?/AU

     FILE 'CAOLD' ENTERED AT 09:46:38 ON 23 APR 2004

=> s l10
L14          1 L10

=> d l14, all, 1

L14  ANSWER 1 OF 1  CAOLD  COPYRIGHT 2004 ACS on STN
AN   CA51:4559f  CAOLD
TI   antitumor substances - (I) effect of org. Se compds. on the Ehrlich
     ascites carcinoma
AU   Takeda, Kenichi; Nishimura, H.; Shimaoka, N.; Noguchi, R.; Nakajima, K.
IT    273-15-4    273-91-6   1123-91-7   2818-88-4 114353-69-4 118802-56-5
     119248-56-5 121621-29-2 121623-43-6


=> fil reg; d acc 119248-56-5; fil CAOLD

FILE 'REGISTRY' ENTERED AT 09:46:53 ON 23 APR 2004
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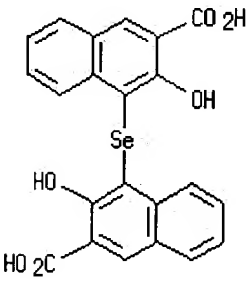
ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 119248-56-5 REGISTRY
CN 2-Naphthoic acid, 4,4'-selenobis[3-hydroxy- (6CI) (CA INDEX NAME)
MF C22 H14 O6 Se
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 09:46:53 ON 23 APR 2004

=> **file reg**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	515.50

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.85

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 23 APR 2004
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7
DICTIONARY FILE UPDATES: 21 APR 2004 HIGHEST RN 676437-01-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L15     STRUCTURE UPLOADED

=> l15
L15 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d l15
L15 HAS NO ANSWERS
L15             STR

=> s l15
SAMPLE SEARCH INITIATED 09:47:51 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    949 TO ITERATE

100.0% PROCESSED     949 ITERATIONS                                  49 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        17132 TO    20828
PROJECTED ANSWERS:             560 TO     1400

L16          49 SEA SSS SAM L15

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DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED -  18609 TO ITERATE

100.0% PROCESSED   18609 ITERATIONS                              1148 ANSWERS
SEARCH TIME: 00.00.01

L17        1148 SEA SSS FUL L15

=> d his

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     FILE 'REGISTRY' ENTERED AT 09:32:24 ON 23 APR 2004
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L2            0 S L1
L3            0 S L1 FULL

     FILE 'BEILSTEIN' ENTERED AT 09:42:55 ON 23 APR 2004
L4            0 S L1

     FILE 'REGISTRY' ENTERED AT 09:43:07 ON 23 APR 2004
L5              STRUCTURE UPLOADED
L6            0 S L5
L7            0 S L5 FULL
L8              STRUCTURE UPLOADED
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L9             0 S L8
L10           10 S L8 FULL

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L12            0 S L11 AND BERNARDON, J?/AU
L13            0 S L11 AND DIAZ, P?/AU

     FILE 'CAOLD' ENTERED AT 09:46:38 ON 23 APR 2004
L14            1 S L10

     FILE 'REGISTRY' ENTERED AT 09:46:53 ON 23 APR 2004

     FILE 'CAOLD' ENTERED AT 09:46:53 ON 23 APR 2004

     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 23 APR 2004
L15              STRUCTURE UPLOADED
L16           49 S L15
L17         1148 S L15 FULL

=>
L18      STRUCTURE UPLOADED

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L18 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
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L18 HAS NO ANSWERS
L18              STR

=> s l18
SAMPLE SEARCH INITIATED 09:48:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     827 TO ITERATE

100.0% PROCESSED      827 ITERATIONS                                46 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        14815 TO    18265
PROJECTED ANSWERS:             514 TO     1326

L19           46 SEA SSS SAM L18

=> s l18 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:48:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  16454 TO ITERATE

100.0% PROCESSED   16454 ITERATIONS                             1072 ANSWERS
SEARCH TIME: 00.00.01

L20         1072 SEA SSS FUL L18

=> d his
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     (FILE 'HOME' ENTERED AT 09:28:14 ON 23 APR 2004)

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L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FULL

     FILE 'BEILSTEIN' ENTERED AT 09:42:55 ON 23 APR 2004
L4           0 S L1

     FILE 'REGISTRY' ENTERED AT 09:43:07 ON 23 APR 2004
L5             STRUCTURE UPLOADED
L6           0 S L5
L7           0 S L5 FULL
L8             STRUCTURE UPLOADED
L9           0 S L8
L10         10 S L8 FULL

     FILE 'HCAPLUS' ENTERED AT 09:45:49 ON 23 APR 2004
L11          7 S L10
L12          0 S L11 AND BERNARDON, J?/AU
L13          0 S L11 AND DIAZ, P?/AU

     FILE 'CAOLD' ENTERED AT 09:46:38 ON 23 APR 2004
L14          1 S L10

     FILE 'REGISTRY' ENTERED AT 09:46:53 ON 23 APR 2004

     FILE 'CAOLD' ENTERED AT 09:46:53 ON 23 APR 2004

     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 23 APR 2004
L15            STRUCTURE UPLOADED
L16         49 S L15
L17       1148 S L15 FULL
L18            STRUCTURE UPLOADED
L19         46 S L18
L20       1072 S L18 FULL

=> s 120 not l10
L21       1072 L20 NOT L10

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                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   311.26     826.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -4.85

FILE 'HCAPLUS' ENTERED AT 09:49:02 ON 23 APR 2004
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FILE COVERS 1907 - 23 Apr 2004 VOL 140 ISS 18
FILE LAST UPDATED: 22 Apr 2004 (20040422/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

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L22 570 L21

=> **s l22 and bernardon, j?/au**
68 BERNARDON, J?/AU
L23 1 L22 AND BERNARDON, J?/AU

=> **d l23, ibib abs fhitstr, 1**

L23 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

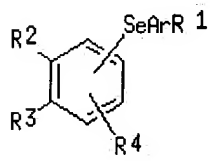
Full Text | Citing References

ACCESSION NUMBER: 1999:811209 HCAPLUS
DOCUMENT NUMBER: 132:35910
TITLE: Preparation of diaryl selenide compounds and their use in human or veterinary medicine and in cosmetics
INVENTOR(S): **Bernardon, Jean-Michel**; Diaz, Philippe
PATENT ASSIGNEE(S): Galderma Research & Development, S.N.C., Fr.
SOURCE: PCT Int. Appl., 81 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9965872	A1	19991223	WO 1999-FR1389	19990611
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2779720	A1	19991217	FR 1998-7439	19980612
FR 2779720	B1	20020816		
CA 2334843	AA	19991223	CA 1999-2334843	19990611
AU 9940491	A1	20000105	AU 1999-40491	19990611
AU 753187	B2	20021010		
EP 1086080	A1	20010328	EP 1999-923723	19990611
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9911833	A	20010925	BR 1999-11833	19990611
JP 2002518371	T2	20020625	JP 2000-554699	19990611

ZA 2000006518	A	20010730	ZA 2000-6518		20001110
NO 2000006337	A	20010212	NO 2000-6337		20001212
PRIORITY APPLN. INFO.:			FR 1998-7439	A	19980612
			WO 1999-FR1389	W	19990611

OTHER SOURCE(S): MARPAT 132:35910
GI

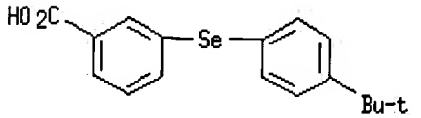


I

AB The invention concerns novel diaryl selenide compds. corresponding to I and their geometric and optical isomers and salts and the use thereof in pharmaceutical compns. in human or veterinary medicine (in the treatment of dermatol., rheumatic, cardiovascular and ophthalmol. pathologies in particular), or in cosmetic compns. In I, R1 = Me, CH2OR5 (R5 = H, lower alkyl, C(O)R10 (R10 = lower alkyl)), C(O)R6 (R6 = H, lower alkyl, OR12 (R12 = H, lower alkyl, aryl, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl), NR'R'' (R'/R'' = H, lower alkyl, aryl possibly substituted, amino acid fragment; R' and R'' together with N form a heterocycle)); Ar = R7-substituted benzene or pyridine diradical (R7 = H, halogen, lower alkyl, nitro, OR13 (R13 = H, lower alkyl), polyether radical, NR14R15 (R14/R15 = H, lower alkyl)), diradicals of furan, thiophene or thiazole; R2/R3 = H, tBu, 1-methylcyclohexyl, 1-adamantyl, OR8 (R8 = H, lower alkyl, aryl possibly substituted, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl, lower alkyl), polyether radical, where at least one of R2 or R3 = tBu, 1-methylcyclohexyl, 1-adamantyl; R2 and R3 may together with an adjacent arom. ring form a satd. 5- or 6-membered ring possibly substituted by Me groups and/or possibly interrupted by O or S; R4 = H, halogen, lower alkyl, OR9 (R9 = H, lower alkyl, aryl possibly substituted, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl, lower alkyl, (CH2)nCO2R16 (R16 = H, lower alkyl; n = 1-12), (CH2)nX (X = halogen)), polyether radical, C(O)R10. Although the method of prepn. is not claimed, 70 example prepns. are included. In a typical prepn., a haloarene (e.g. 2-bromo-5,6,7,8-tetrahydro-3,5,5,8,8-pentamethylnaphthalene) is successively reacted with tBuLi in THF, Se, and NaOH in EtOH to give a diselenide, which is cleaved with NaBH4 in EtOH to give the Na salt of an areneselenol, which is undergoes metathesis with IR1 or BrR1 (e.g. Et 4-iodobenzoate) in the presence of NiBr2py2 in EtOH to give I (e.g. Et 4-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-ylselenenyl)benzoate).

IT **252352-01-5P**, 3-(4-tert-Butylphenylselenenyl)benzoic acid
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of diaryl selenide compds. and use in human or veterinary medicine and in cosmetics)

RN 252352-01-5 HCAPLUS
CN Benzoic acid, 3-[[4-(1,1-dimethylethyl)phenyl]seleno]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> file uspatful
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     7.12     833.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -0.69      -5.54

FILE 'USPATFULL' ENTERED AT 09:49:35 ON 23 APR 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 22 Apr 2004 (20040422/PD)
FILE LAST UPDATED: 22 Apr 2004 (20040422/ED)
HIGHEST GRANTED PATENT NUMBER: US6725463
HIGHEST APPLICATION PUBLICATION NUMBER: US2004078858
CA INDEXING IS CURRENT THROUGH 22 Apr 2004 (20040422/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 22 Apr 2004 (20040422/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2004
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2004

>>>  USPAT2 is now available.  USPATFULL contains full text of the     <<<
>>>  original, i.e., the earliest published granted patents or         <<<
>>>  applications.  USPAT2 contains full text of the latest US         <<<
>>>  publications, starting in 2001, for the inventions covered in     <<<
>>>  USPATFULL.  A USPATFULL record contains not only the original     <<<
>>>  published document but also a list of any subsequent              <<<
>>>  publications.  The publication number, patent kind code, and      <<<
>>>  publication date for all the US publications for an invention     <<<
>>>  are displayed in the PI (Patent Information) field of USPATFULL   <<<
>>>  records and may be searched in standard search fields, e.g., /PN, <<<
>>>  /PK, etc.                                                         <<<

>>>  USPATFULL and USPAT2 can be accessed and searched together        <<<
>>>  through the new cluster USPATALL.  Type FILE USPATALL to          <<<
>>>  enter this cluster.                                               <<<
>>>                                                                    <<<
>>>  Use USPATALL when searching terms such as patent assignees,       <<<
>>>  classifications, or claims, that may potentially change from      <<<
>>>  the earliest to the latest publication.                           <<<

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=> file uspatfull
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                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     1.35     835.23

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                     0.00      -5.54

FILE 'USPATFULL' ENTERED AT 09:49:39 ON 23 APR 2004
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 22 Apr 2004 (20040422/PD)
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FILE LAST UPDATED: 22 Apr 2004 (20040422/ED)
HIGHEST GRANTED PATENT NUMBER: US6725463
HIGHEST APPLICATION PUBLICATION NUMBER: US2004078858
CA INDEXING IS CURRENT THROUGH 22 Apr 2004 (20040422/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 22 Apr 2004 (20040422/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2004
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2004

>>>  USPAT2 is now available.  USPATFULL contains full text of the     <<<
>>>  original, i.e., the earliest published granted patents or         <<<
>>>  applications.  USPAT2 contains full text of the latest US         <<<
>>>  publications, starting in 2001, for the inventions covered in     <<<
>>>  USPATFULL.  A USPATFULL record contains not only the original     <<<
>>>  published document but also a list of any subsequent              <<<
>>>  publications.  The publication number, patent kind code, and      <<<
>>>  publication date for all the US publications for an invention     <<<
>>>  are displayed in the PI (Patent Information) field of USPATFULL   <<<
>>>  records and may be searched in standard search fields, e.g., /PN, <<<
>>>  /PK, etc.                                                         <<<

>>>  USPATFULL and USPAT2 can be accessed and searched together        <<<
>>>  through the new cluster USPATALL.  Type FILE USPATALL to          <<<
>>>  enter this cluster.                                               <<<
>>>                                                                    <<<
>>>  Use USPATALL when searching terms such as patent assignees,       <<<
>>>  classifications, or claims, that may potentially change from      <<<
>>>  the earliest to the latest publication.                           <<<

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=> d his

     (FILE 'HOME' ENTERED AT 09:28:14 ON 23 APR 2004)

     FILE 'REGISTRY' ENTERED AT 09:32:24 ON 23 APR 2004
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FULL

     FILE 'BEILSTEIN' ENTERED AT 09:42:55 ON 23 APR 2004
L4           0 S L1

     FILE 'REGISTRY' ENTERED AT 09:43:07 ON 23 APR 2004
L5             STRUCTURE UPLOADED
L6           0 S L5
L7           0 S L5 FULL
L8             STRUCTURE UPLOADED
L9           0 S L8
L10         10 S L8 FULL

     FILE 'HCAPLUS' ENTERED AT 09:45:49 ON 23 APR 2004
L11          7 S L10
L12          0 S L11 AND BERNARDON, J?/AU
L13          0 S L11 AND DIAZ, P?/AU

     FILE 'CAOLD' ENTERED AT 09:46:38 ON 23 APR 2004
L14          1 S L10

     FILE 'REGISTRY' ENTERED AT 09:46:53 ON 23 APR 2004
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     FILE 'CAOLD' ENTERED AT 09:46:53 ON 23 APR 2004

     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 23 APR 2004
L15             STRUCTURE UPLOADED
L16          49 S L15
L17        1148 S L15 FULL
L18             STRUCTURE UPLOADED
L19          46 S L18
L20        1072 S L18 FULL
L21        1072 S L20 NOT L10

     FILE 'HCAPLUS' ENTERED AT 09:49:02 ON 23 APR 2004
L22         570 S L21
L23           1 S L22 AND BERNARDON, J?/AU

     FILE 'USPATFULL' ENTERED AT 09:49:35 ON 23 APR 2004

     FILE 'USPATFULL' ENTERED AT 09:49:39 ON 23 APR 2004

=> s l21
L24          45 L21

=> s l24 and bernardon, j?/au
            90 BERNARDON, J?/AU
L25          0 L24 AND BERNARDON, J?/AU

=> s l24 and diaz, p?/au
            27 DIAZ, P?/AU
L26          0 L24 AND DIAZ, P?/AU

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COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               22.79     858.02

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00      -5.54

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FILE COVERS 1907 - 23 Apr 2004  VOL 140 ISS 18
FILE LAST UPDATED: 22 Apr 2004  (20040422/ED)

 This file contains CAS Registry Numbers for easy and accurate
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substance identification.

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=> d his

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     FILE 'REGISTRY' ENTERED AT 09:32:24 ON 23 APR 2004
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FULL

     FILE 'BEILSTEIN' ENTERED AT 09:42:55 ON 23 APR 2004
L4           0 S L1

     FILE 'REGISTRY' ENTERED AT 09:43:07 ON 23 APR 2004
L5             STRUCTURE UPLOADED
L6           0 S L5
L7           0 S L5 FULL
L8             STRUCTURE UPLOADED
L9           0 S L8
L10         10 S L8 FULL

     FILE 'HCAPLUS' ENTERED AT 09:45:49 ON 23 APR 2004
L11          7 S L10
L12          0 S L11 AND BERNARDON, J?/AU
L13          0 S L11 AND DIAZ, P?/AU

     FILE 'CAOLD' ENTERED AT 09:46:38 ON 23 APR 2004
L14          1 S L10

     FILE 'REGISTRY' ENTERED AT 09:46:53 ON 23 APR 2004

     FILE 'CAOLD' ENTERED AT 09:46:53 ON 23 APR 2004

     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 23 APR 2004
L15            STRUCTURE UPLOADED
L16         49 S L15
L17       1148 S L15 FULL
L18            STRUCTURE UPLOADED
L19         46 S L18
L20       1072 S L18 FULL
L21       1072 S L20 NOT L10

     FILE 'HCAPLUS' ENTERED AT 09:49:02 ON 23 APR 2004
L22        570 S L21
L23          1 S L22 AND BERNARDON, J?/AU

     FILE 'USPATFULL' ENTERED AT 09:49:35 ON 23 APR 2004

     FILE 'USPATFULL' ENTERED AT 09:49:39 ON 23 APR 2004
L24         45 S L21
L25          0 S L24 AND BERNARDON, J?/AU
L26          0 S L24 AND DIAZ, P?/AU

     FILE 'HCAPLUS' ENTERED AT 09:50:13 ON 23 APR 2004

=> s l21 and diaz, p?/au
          570 L21
          602 DIAZ, P?/AU
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L27           2 L21 AND DIAZ, P?/AU

=> s l27 not l23
L28           1 L27 NOT L23

=> d l28, ibib abs fhitstr, 1

L28  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2004 ACS on STN
```

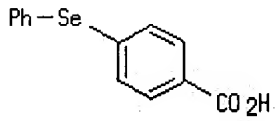
Full Text | Citing References

ACCESSION NUMBER: 2000:338377 HCAPLUS
DOCUMENT NUMBER: 133:89593
TITLE: Solution-Phase Synthesis of Diaryl Selenides Using Polymer-Supported Borohydride
AUTHOR(S): Millois, Corinne; **Diaz, Philippe**
CORPORATE SOURCE: GALDERMA RD, Sophia-Antipolis, F06902, Fr.
SOURCE: Organic Letters (2000), 2(12), 1705-1708
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:89593

operability

AB A new series of selenium-contg. diaryl retinoids have been prepd. by a new direct nickel(II)-catalyzed coupling of a diselenide with an iodoaryl in the presence of polymer-supported borohydride. Thus, (bpy)2NiBr2-catalyzed coupling reaction of bis(4-chlorophenyl) diselenide with Me 3-iodobenzoate in the presence of Aldrich 32,864-2 resin in THF/MeOH gave 84% 4-ClC6H4SeC6H4CO2Me-2.

IT **106206-61-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 106206-61-5 HCAPLUS
CN Benzoic acid, 4-(phenylseleno)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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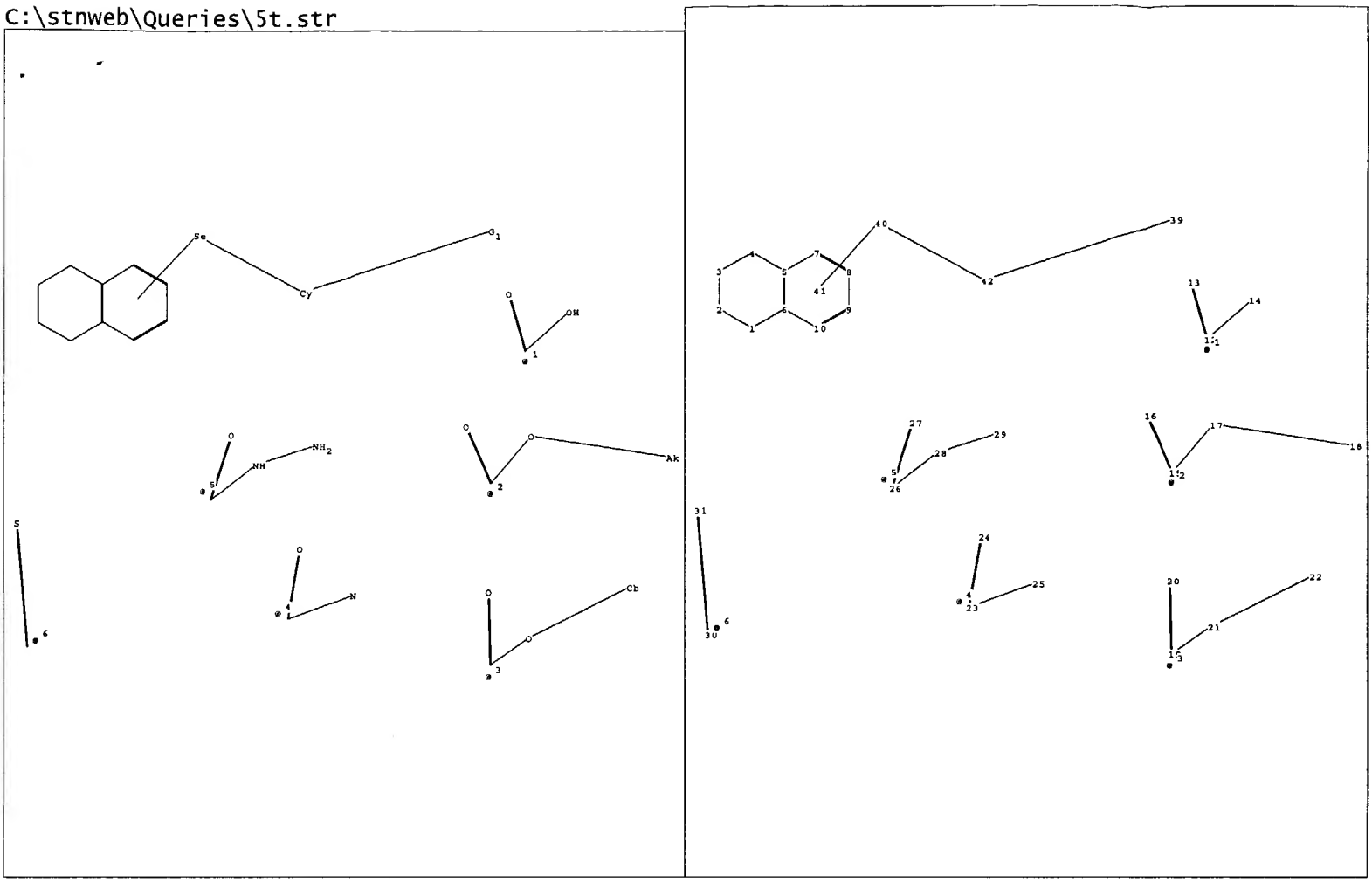

chain nodes :
12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 39 40 42
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
12-13 12-14 15-16 15-17 17-18 19-20 19-21 21-22 23-24 23-25 26-27 26-28 28-29
30-31 39-42 40-42
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
15-16 15-17 17-18 19-20 19-21 23-24 23-25 26-27 26-28 30-31 39-42 40-42
exact bonds :
1-2 1-6 2-3 3-4 4-5 21-22 28-29
normalized bonds :
5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-14
isolated ring systems :
containing 1 :

G1:[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom

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 NEWS  1            Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2            "Ask CAS" for self-help around the clock
 NEWS  3  JAN 27    Source of Registration (SR) information in REGISTRY updated
                    and searchable
 NEWS  4  JAN 27    A new search aid, the Company Name Thesaurus, available in
                    CA/CAplus
 NEWS  5  FEB 05    German (DE) application and patent publication number format
                    changes
 NEWS  6  MAR 03    MEDLINE and LMEDLINE reloaded
 NEWS  7  MAR 03    MEDLINE file segment of TOXCENTER reloaded
 NEWS  8  MAR 03    FRANCEPAT now available on STN
 NEWS  9  MAR 29    Pharmaceutical Substances (PS) now available on STN
 NEWS 10  MAR 29    WPIFV now available on STN
 NEWS 11  MAR 29    No connect hour charges in WPIFV until May 1, 2004
 NEWS 12  MAR 29    New monthly current-awareness alert (SDI) frequency in RAPRA

 NEWS EXPRESS  MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 13 APRIL 2004
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 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
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FILE 'HOME' ENTERED AT 15:15:40 ON 23 APR 2004

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

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STRUCTURE FILE UPDATES:   21 APR 2004  HIGHEST RN 676437-01-7
DICTIONARY FILE UPDATES:  21 APR 2004  HIGHEST RN 676437-01-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
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```

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1 STRUCTURE UPLOADED

=> **l1**
L1 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> **d l1**
L1 HAS NO ANSWERS
L1 STR

=> **s l1**
SAMPLE SEARCH INITIATED 15:18:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 33 TO 447
PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> **s l1 full**
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:**y**
FULL SEARCH INITIATED 15:18:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 449 TO ITERATE

100.0% PROCESSED 449 ITERATIONS 62 ANSWERS
SEARCH TIME: 00.00.01

L3 62 SEA SSS FUL L1

=> **file hcaplus**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	157.10	157.31

FILE 'HCAPLUS' ENTERED AT 15:18:38 ON 23 APR 2004
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FILE COVERS 1907 - 23 Apr 2004 VOL 140 ISS 18
FILE LAST UPDATED: 22 Apr 2004 (20040422/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> **s l3**
L4 2 L3

=> **d l4, ibib abs fhitstr, 1-2**

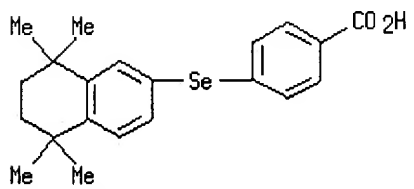
L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:338377 HCAPLUS
DOCUMENT NUMBER: 133:89593
TITLE: Solution-Phase Synthesis of Diaryl Selenides Using Polymer-Supported Borohydride
AUTHOR(S): Millois, Corinne; Diaz, Philippe
CORPORATE SOURCE: GALDERMA RD, Sophia-Antipolis, F06902, Fr.
SOURCE: Organic Letters (2000), 2(12), 1705-1708
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:89593

AB A new series of selenium-contg. diaryl retinoids have been prepd. by a new direct nickel(II)-catalyzed coupling of a diselenide with an iodoaryl in the presence of polymer-supported borohydride. Thus, (bpy)2NiBr2-catalyzed coupling reaction of bis(4-chlorophenyl) diselenide with Me 3-iodobenzoate in the presence of Aldrich 32,864-2 resin in THF/MeOH gave 84% 4-ClC6H4SeC6H4CO2Me-2.

IT **252352-07-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 252352-07-1 HCAPLUS
CN Benzoic acid, 4-[(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)seleno]- (9CI) (CA INDEX NAME)



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L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:811209 HCAPLUS
DOCUMENT NUMBER: 132:35910
TITLE: Preparation of diaryl selenide compounds and their use in human or veterinary medicine and in cosmetics
INVENTOR(S): Bernardon, Jean-Michel; Diaz, Philippe
PATENT ASSIGNEE(S): Galderma Research & Development, S.N.C., Fr.
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FAMILY ACC. NUM. COUNT: 1
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WO 9965872	A1	19991223	WO 1999-FR1389	19990611
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2779720	A1	19991217	FR 1998-7439	19980612
FR 2779720	B1	20020816		
CA 2334843	AA	19991223	CA 1999-2334843	19990611
AU 9940491	A1	20000105	AU 1999-40491	19990611
AU 753187	B2	20021010		
EP 1086080	A1	20010328	EP 1999-923723	19990611
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9911833	A	20010925	BR 1999-11833	19990611
JP 2002518371	T2	20020625	JP 2000-554699	19990611
ZA 2000006518	A	20010730	ZA 2000-6518	20001110
NO 2000006337	A	20010212	NO 2000-6337	20001212

PRIORITY APPLN. INFO.: FR 1998-7439 A 19980612
WO 1999-FR1389 W 19990611

OTHER SOURCE(S): MARPAT 132:35910
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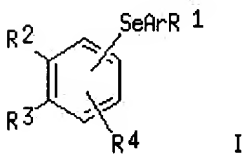


I

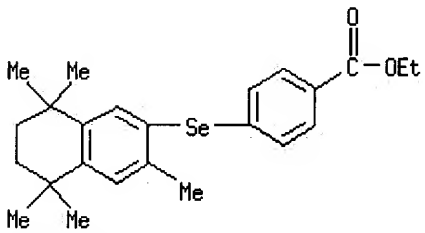
AB The invention concerns novel diaryl selenide compds. corresponding to I and their geometric and optical isomers and salts and the use thereof in pharmaceutical compns. in human or veterinary medicine (in the treatment of dermatol., rheumatic, cardiovascular and ophthalmol. pathologies in particular), or in cosmetic compns. In I, R1 = Me, CH2OR5 (R5 = H, lower alkyl, C(O)R10 (R10 = lower alkyl)), C(O)R6 (R6 = H, lower alkyl, OR12

(R12 = H, lower alkyl, aryl, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl), NR'R'' (R'/R'' = H, lower alkyl, aryl possibly substituted, amino acid fragment; R' and R'' together with N form a heterocycle)); Ar = R7-substituted benzene or pyridine diradical (R7 = H, halogen, lower alkyl, nitro, OR13 (R13 = H, lower alkyl), polyether radical, NR14R15 (R14/R15 = H, lower alkyl)), diradicals of furan, thiophene or thiazole; R2/R3 = H, tBu, 1-methylcyclohexyl, 1-adamantyl, OR8 (R8 = H, lower alkyl, aryl possibly substituted, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl, lower alkyl), polyether radical, where at least one of R2 or R3 = tBu, 1-methylcyclohexyl, 1-adamantyl; R2 and R3 may together with an adjacent arom. ring form a satd. 5- or 6-membered ring possibly substituted by Me groups and/or possibly interrupted by O or S; R4 = H, halogen, lower alkyl, OR9 (R9 = H, lower alkyl, aryl possibly substituted, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl, lower alkyl, (CH2)nCO2R16 (R16 = H, lower alkyl; n = 1-12), (CH2)nX (X = halogen)), polyether radical, C(O)R10. Although the method of prepn. is not claimed, 70 example prepns. are included. In a typical prepn., a haloarene (e.g. 2-bromo-5,6,7,8-tetrahydro-3,5,5,8,8-pentamethylnaphthalene) is successively reacted with tBuLi in THF, Se, and NaOH in EtOH to give a diselenide, which is cleaved with NaBH4 in EtOH to give the Na salt of an areneselenol, which is undergoes metathesis with IR1 or BrR1 (e.g. Et 4-iodobenzoate) in the presence of NiBr2py2 in EtOH to give I (e.g. Et 4-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-ylselenenyl)benzoate).

IT **252351-97-6P**, Ethyl 4-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydronaphthalen-2-ylselenenyl)benzoate
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of diaryl selenide compds. and use in human or veterinary medicine and in cosmetics)

RN 252351-97-6 HCAPLUS

CN Benzoic acid, 4-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)seleno]-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2004
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2004

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